

pide: Petrophysical Interpretation tools for geoDynamic Exploration.

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Software

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Summary

pide is a Python library for calculating geophysical parameters (e.g., electrical conductivity, seismic velocity), employing the results from experimental petrology, mineral/rock physics, and thermomechanical modelling studies. pide can calculate the theoretical electrical conductivity of any Earth material that exists in the literature. pide can also calculate seismic velocity utilising the external 'sister' library SAnTex. Using these theoretical calculations, users can utilise inversion modules to decode geophysical anomalies compositionally or convert thermomechanical models into geophysical observables. With a given spatial mapping of Earth materials, which can preferentially be loaded from a thermomechanical model, pide can be used to build synthetic electrical conductivity and seismic velocity models and generate gravity and magnetic anomalies. Moreover, pide is built as a modular tool, so users can easily build their functions.

Statement of need

Given the inherent heterogeneity and complexity of Earth systems, geophysical tomographies often yield complex 2D and 3D images that are challenging to interpret. To enhance their interpretations, researchers commonly turn to experimental petrology and mineral physics, covering various geophysical properties, including electrical conductivity, magnetic susceptibility, seismic velocity, and rheology. These properties are sensitive to phase transitions, partial melting, major and trace elements partitioning, mineral solubilities, and phase-mixing models. Numerous specialized tools have been designed to address specific properties, many of which feature graphical interfaces [e.g.,MATE; Özaydın & Selway (2020); Abers & Hacker (2016)] or are accessible through web-based applications like sigmelts (Pommier & Le-Trong, 2011). In this context, pide is a solution fulfilling the need for a versatile library capable of facilitating petrophysical calculations across a range of properties and supporting the creation of specific scientific tools. Beyond this, pide aims to host toolkits tailored for specific purposes, such as constructing realistic, petrophysically constrained synthetic models and converting numerical plate tectonic models into synthetic geophysical tomographies.

Library modules and methods

The general workflow diagram of the library can ben seen in Figure 1. The library has three main classes used in these calculations: pide, material and model.

pide is the main class in which the electrical conductivity and seismic-related observables

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are calculated. In order to achieve this, the relevant parameters have to be defined in the pide object with the associated functions (e.g., composition, water content, interconnectivity). Just using the pide class, for instance, the user can make a figure of all calculations of all the olivine electrical conductivity and seismic velocity models for olivine. While experimental parameters for electrical conductivity parameters are defined and calculated within the pide, seismic velocities of given Earth materials are calculated through SAnTex library automatically.

material is the class that can be specified as a holder of pre-defined material properties. For instance, one can create a Lherzolite material by mixing specific modal proportions of olivine (ol), orthopyroxene (opx), clinopyroxene (cpx) and garnet (gt), how these constituents are interconnected, or how water behaves among them.



Figure 1: Workflow Chart for pide

The model class, on the other hand, is where a collection of material objects can be appended with specific positions indexed in 3D space. model is also where the user can calculate the magnetic and gravitational anomalies solely since these observables are dependent on the position of the materials and assigned magnetic and density parameters only. pide can generate synthetic data for magnetic and gravitational anomalies utilising the harmonica library (Fatiando a Terra Project et al., 2024).

pide can generate synthetic electric conductivity and seismic velocity models that can be saved as input files for commonly used magnetotelluric modelling algorithms ModEM (Kelbert et al., 2014) and Mare2DEM (Key, 2016). Users then can generate synthetic data using the algorithms provided by these software packages. These functions can be found in the mt module.

pide also comes with several modules that can exploit the library classes. 'model_modifier' functions. Utilising 'model_modifier' functions, pide can convert a thermomechanical model into a 'realistic' synthetic electrical conductivity model (Figure 2). Details of this conversion can be seen in the Notebook named 10_2D_Underworld_Conversion_II_Narrow_Rift.ipynb. inversion module, on the other hand, can be utilised to invert for specific input parameters (e.g., composition, melt content, mineral interconnection) that fit outputs of geophysical models. Currently, the inversion module supports a single-parameter optimisation method with a line search algorithm. However, in future releases, we will explore creating an ensemble of compositional solutions via a probabilistic approach.





Figure 2: Example of pide is being used for conversion of a thermoemchanical model into a synthetic MT model.

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